

A BEM model for heat flux exchange between particles and fluid

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Abstract - This study is concerned with the problem of two-way coupled simulations of multiphase flows within an Eulerian-Lagrange framework. For a point-wise particles the standard method to introduce the Lagrangian particles as sources into the Eulerian mesh is the particle-in-cell (PIC) method. In this study, we present a boundary element method (BEM) model instead and show that the novel BEM model gives superior results when particles are not located close to the mesh nodes. We introduce a critical distance from the mesh node, which separates the domain volume, where the BEM model can be used and the volume, where the PIC model should be used. The results show that the BEM model can be used in about 90% - 99% of the volume depending on the mesh used.

Keywords: Boundary element method, particle-in-cell, critical distance, point-wise particles.

1. Introduction

Multiphase flows are fundamental in process technology. Their two main aspects are either mixture separation or, in contrary, making a mixture out of two pure substances as homogeneous as possible. Coupling between phases in multiphase flow can be modelled in different ways. Assuming there is only a significant force in the direction from carrier phase onto particulate phase, we call a flow 1-way coupled. In a case there is a mutual interaction between the two phases, we call it 2-way coupled flow [1]. The 4-way coupled flow considered also collisions between the particles. According to ratio of volume of both phases we distinguish dense and dilute flows. Characteristics of dilute flow is, that the most important forces that occur, are interacting forces between two phases, while for dense flows the main flow characteristics come from the particle collisions. The dilute flows are generally modelled using Euler-Lagrange models [2]. The accuracy of the Euler-Lagrange model depends on the accuracy of the interphase momentum/heat transfer between particle and mesh vertices. Interphase exchange is usually modelled using Particle-in-cell method, introduced firstly by Evans and Harlow [3]. Method is based on volume averaging across the computation cell, in which particle is located. First disadvantage of the method is that volume averaging does not have a physical background and the second one, that it is strongly dependent on mesh grid [4]. Fluid is most commonly modelled by the finite volume method, which is coupled with Lagrangian particle tracking and PIC for momentum/heat exchange. Our CFD solver uses the Boundary-Domain Integral Method BDIM [5], which has an unique advantage when handling point sources. In this paper, we will demonstrate how to use the BEM to derive a novel heat/momentum exchange model.

2. Governing equations

As a model problem we consider heat diffusion from a point-wise particle with a constant heat source ζ . The chosen phenomenon is representative enough and the analytical solution in an unbounded domain is known. The dimensionless differential equation describing the phenomenon is:

$$\frac{\partial T}{\partial \tau} - \nabla^2 T = \zeta \delta(\vec{r}, \vec{p}) \quad (1.a)$$

where τ represents the dimensionless time, \vec{r} is the location vector, \vec{p} is the particle position and T is dimensionless temperature. Alternatively, we can model the particle as a constant volume source of energy within a single mesh element,

$$\frac{\partial T}{\partial \tau} - \nabla^2 T = \frac{\zeta}{V_e} \quad (1.b)$$

where V_e is the volume of the mesh element, in which the particle is located. This is the basis of the standard PIC method. Eq. (1.a) can be transformed into an integral equation using the Green's clause as [6]:

$$c(\vec{\xi})T(\vec{\xi}) + \int_{\Gamma} T(\vec{r}) \vec{q}^*(\vec{\xi}, \vec{r}) \cdot d\vec{\Gamma} = \int_{\Gamma} u^*(\vec{\xi}, \vec{r}) \vec{q} \cdot d\vec{\Gamma} - \int_{\Omega} \left(\frac{\partial T(\vec{r})}{\partial \tau} \right) u^*(\vec{\xi}, \vec{r}) d\Omega + \int_{\Omega} \zeta \delta(\vec{r}, \vec{p}) u^*(\vec{\xi}, \vec{r}) d\Omega, \quad (2)$$

Where $\vec{\xi}$ is the location vector of the source point, $u^*(\vec{\xi}, \vec{r})$ is the fundamental solution of the Laplace equation, $q^*(\vec{\xi}, \vec{r})$ is the gradient of the fundamental solution, $c(\vec{\xi})$ the free term coefficient and $\vec{q} = \vec{\nabla}T$. The $\vec{\Gamma}$ and Ω are domain boundary and the domain, respectively. When employing BDIM we mesh the domain with domain elements. Eq. (2) is used on each element in via compatibility boundary conditions, a system of linear equations for temperature and its flux is obtained. Further details about BDIM are given in [7].

Heat flux exchange between particles and the fluid is modelled by the last term on the right hand side of (2). Due to the properties of the Kronecker delta functions, we may write

$$\int_{\Omega} \zeta \delta(\vec{r}, \vec{p}) u^*(\vec{\xi}, \vec{r}) d\Omega = \zeta u^*(\vec{p}, \vec{r}) \quad (3)$$

and thus avoid domain integration. Boundary domain integral method thus enables us to implement heat exchange from particles to fluid by simply summing the contribution of all particles using the formula given in (3). The drawback of this approach is the singularity of u^* , which occurs when the particle is located close to a mesh node.

The interphase heat exchange in PIC method takes place inside of the element, in which the particle is located. We model the particle as a constant heat source within the mesh element in which they are located. Transforming Eq. (1.b) into integral form, we obtain:

$$c(\vec{\xi})T(\vec{\xi}) + \int_{\Gamma} T(\vec{r}) \vec{q}^*(\vec{\xi}, \vec{r}) \cdot d\vec{\Gamma} = \int_{\Gamma} u^*(\vec{\xi}, \vec{r}) \vec{q} \cdot d\vec{\Gamma} - \int_{\Omega} \left(\frac{\partial T(\vec{r})}{\partial \tau} \right) u^*(\vec{\xi}, \vec{r}) d\Omega + \frac{\zeta}{V_e} \int_{\Omega_e} u^*(\vec{\xi}, \vec{r}) d\Omega. \quad (4)$$

Representation (4) requires the calculation of the domain integral due to particle presence and does not consider the exact location of the particle. Both of these facts are seen as drawbacks of the PIC method as compared to the newly proposed BEM method (3). To facilitate the comparison of the results we define the RMS norm as

$$l_{RMS} = \sqrt{\frac{\sum_{i=1}^N (T_{ana} - T_{num})^2}{\sum_{i=1}^N T_{ana}^2}}, \quad (5)$$

where T_{ana} is the result obtained by the analytical calculation and the T_{num} is the result of the calculation using either BEM or PIC.

3. Numerical example

We consider a cubical domain $(0,1)^3$ and place one particle inside, which emits heat with source ζ . Initially, the domain is at $T=0$. We prescribe Dirichlet boundary conditions on the boundary of the domain using the known analytical solution of this problem [8]

$$T_{ana}(r, \tau) = \frac{\zeta}{4\pi r} \operatorname{erfc}\left(\frac{r}{2\sqrt{\tau}}\right). \quad (6)$$

The domain is meshed using cubical elements having quadratic interpolation of functions and linear interpolation of flux. Thus, each mesh element has 27 function nodes and 24 flux nodes. Due to symmetry, we place the particles only in 1/8 of the cell without loss of generality (Figure 1a). We run each simulation until $\tau = 10$ and use Eq. (5) to calculate the RMS norm. The simulations were done four times, for each of the two different meshes twice. Firstly, we consider the mesh with regular elements and secondly a mesh with irregular, cuboidally shaped elements. The distribution of elements in the meshes was $4 \times 4 \times 4$ and $8 \times 8 \times 8$ with 64 and 512 elements, respectively. Every simulation had only one particle in the domain. The number of simulations has been $\sim 10^5$. Each particle had a dimensionless heat source of magnitude $\zeta = 10$. The locations of the particles have been defined with use of a geometry modeller – they were placed in a volume of $1/8^{\text{th}}$ of a single element located inside the domain, with no border to domain's surfaces.

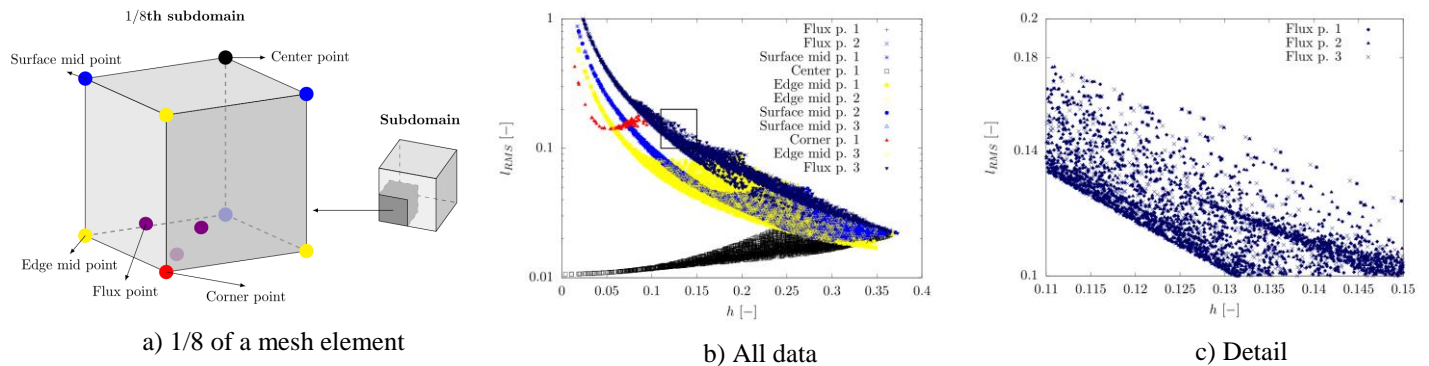


Fig. 1: A view of nodes in 1/8th of a mesh element. Nodes were colour coded by type based on their location (edge, center, surface) (a). Panels (b) and (c) show the RMS norm of the temperature solution versus the distance of the particle to the closest mesh node.

For every simulation the RMS norm l_{RMS} and a distance from the particle to the closest mesh node d have been computed. Since different meshes were used, a new dimensionless parameter was introduced as $h = \frac{d}{\sqrt[3]{V_{element}}}$.

According to the type of the mesh node, closest to the particle position, the results can be divided into five mesh node groups with different characteristics (Figure 1). The first group (violet color) consists of all the flux nodes, the second group (yellow) of the edge mid nodes, third (blue) of the surface mid nodes, the fourth (red) of corner node and the last (black) of center node. Every mesh node inside the group has the same specifics, which is proven by looking at the figure 1c. There are, when observed in detail, all three flux nodes inside the violet group and each of them separately has the same shape as the other two. Thus, we proved that the error of the computed temperature with a specific distance between particle and the mesh node would be of the same order of magnitude, independently of which mesh node of same type is taken.

In Figure 2a we show the relationship between RMS norm l_{RMS} and dimensionless distance for a set of particles, where were located at an approximately equal distance for the edge mid mesh node. The inset panel show that the RMS norm is highest for the particles, for which the second closest mesh node is a flux node.

Considering only worst-case simulations with highest RMS norm values, we prepared Figure 2b out of all simulation data, which was shown in Figure 1b. We applied a moving average filter to obtain smooth RMS norm versus distance relationship. The dashed line in Figure 1b represents the RMS norm obtained, when using the PIC heat exchange model. For each of the mesh node groups there exists a critical dimensionless distance \hat{h} at which the PIC model outperforms the newly proposed BEM model. The PIC l_{RMS} is constant regardless of the particle position in the mesh element. The critical dimensionless distance \hat{h} is defined as a distance for which the simulation using BEM and PIC heat exchange model have the same l_{RMS} . The critical distance is largest for the flux nodes and smallest for the centre node.

Finally, we plot results obtained using different meshes in the same graph for the comparison (Figure 2c). We observe that a finer mesh, which includes smaller elements, leads results of the same order of magnitude for the particle at the same

dimensionless distance from the mesh nodes. Furthermore, the mesh with irregularly shaped elements also results in RMS norms of the same order of magnitude.

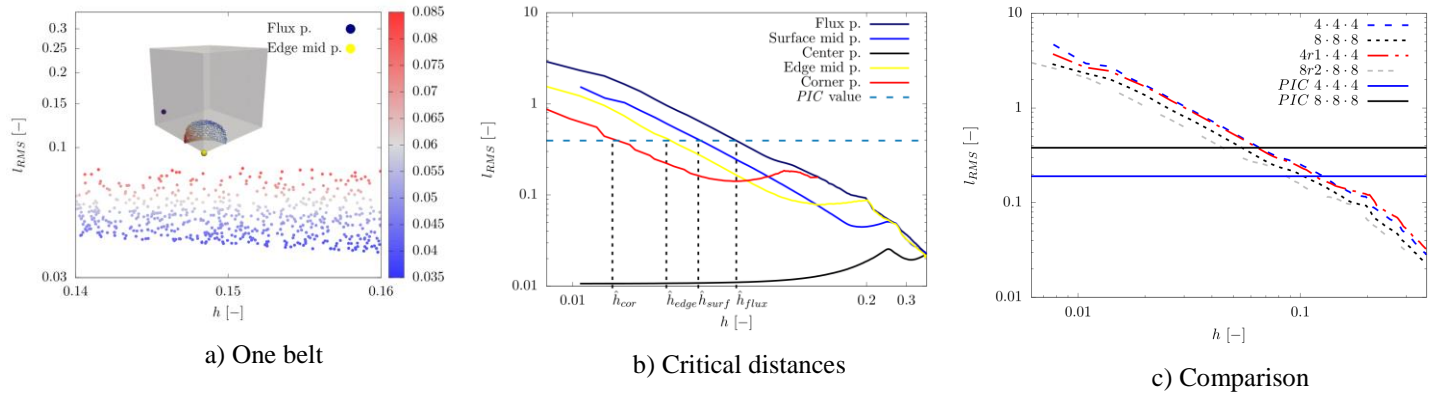


Fig. 2: The particles who have a second closest mesh node nearer than others, have also higher l_{RMS} (a). Worst case error norm versus distance and definition of critical distances \hat{h} (b). Mesh design and number of elements have an impact on the results. (c).

4. Conclusions

We presented a novel model for heat/momentum exchange in Euler-Lagrange simulations of particle laden flows. The presented model uses the properties of the integral representation of the governing equations obtained via Greens clause and with the aid of the fundamental solution of the problem. We compared the developed model with the standard PIC model and discovered the existence of a critical distance between the particle and the mesh nodes, where the new model outperforms the PIC model. The PIC model is superior only in cases, when particle is located very close to the mesh nodes. Results reveal, that the flux mesh node have the highest critical distance. The accuracy of the results depends on the mesh size. The new model yields results of superior accuracy when the particle is located in about 90% of the domain volume.

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